



chain nodes :

7 8 15 17 18 19 20 23 24 25 28 29 31 32 33 34 36 37

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 14

chain bonds :

1-32 2-29 3-28 4-31 5-7 6-33 7-8 7-15 8-9 10-34 12-23 13-36 14-37 17-18 19-20
24-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14

exact/norm bonds :

1-32 2-29 3-28 4-31 6-33 7-8 7-15 8-9 10-34 12-23 13-36 14-37 17-18 24-25

exact bonds :

5-7 19-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14

G1:X,Ak, [*1] , [*2]

G2:H,X,Ak,NO2,CN,Ph

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 23:CLASS 24:CLASS
25:CLASS 28:CLASS 29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 36:CLASS 37:CLASS